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Theory of Optical and Electronic Properties of Clusters and Nanostructures

Period Covered: 07/01/1989 to 06/30/2006

jrc@ices.utexas.edu • **JAMES R. CHELIKOWSKY** • (512) 471-3312

W.A. "Tex" Moncrief Jr. Chair in Computational Materials
Director, Center for Computational Materials Institute for Computational Engineering and Sciences

Professor in the Departments of Physics, Chemical Engineering, and and Chemistry and Biochemistry

Synopsis

The work reported here took place at the University of Minnesota from 07/01/1989 to 06/30/2006. Most of this work focused on computational materials applied to oxides during the first part of this funding period and to nanoscale materials toward the end of the funding period. This funding resulted in three monographs, 36 invited articles or book chapters, 160 articles in refereed journals and 89 invited talks. The funding helped train 13 PhD students and one masters student. The PI received two national research awards for this work. A list of these contributions is presented below.

Recognitions

Professorships

- Neal Amundson Professor, University of Minnesota, 1996.
- Miller Institute Professor, University of California at Berkeley, 1999.

Fellowships

- John Simon Guggenheim Fellowship, 1995-96.
- Fellow of the American Association for the Advancement of Science, 2007. Citation: *For contributions to the basic understanding of properties of materials through theoretical calculations, and for excellence in teaching, lecturing and writing.*

Research Awards

- David Turnbull Lectureship Award, Materials Research Society, 2001.
  Citation: *For his contributions to the fundamental understanding of electronic, optical, mechanical, surface and interface properties of bulk materials and nanostructured semiconductors, ceramics, and metals through ab initio calculations; and for excellence in teaching, lecturing and writing.*

- David Adler Lectureship Award, American Physical Society, 2006.
  Citation: *For his creative and outstanding research in computational materials physics and for his effectiveness in communicating research results through lectures and publications.*

Service Awards

- Outstanding Referee for the American Physical Society, 2008 (lifetime award).

Publications fully or partially supported by the DOE

Books and Monographs

1. J.R. Chelikowsky, and A. Franciosi, Editors: *Electronic Materials: A New Era of Materials Science*, (Springer-Verlag), Vol. 95, 1991.
2. J.R. Chelikowsky, and S.G. Louie, editors: *Quantum Theory of Real Materials*, (Kluwer Press, 1996).
3. E. Shirley, J.R. Chelikowsky, S.G. Louie and G. Martinez, editors: *Optical Properties of Materials*, Materials Research Society Symposium, Vol. 579 (MRS, Warrendale, 2000).

Book Chapters and Invited Articles

1. J.R. Chelikowsky: "Cohesion in Solids," *Encyclopedia of Applied Physics*, ed. G.I. Trigg, (VCH Publishers, AIP, 1992).
2. J.R. Chelikowsky, and M.L. Cohen: "Ab initio Pseudopotentials for Semiconductors," *Handbook on Semiconductors*, Editor: Peter Landsberg, (Elsevier, 1992), Vol. 1, p. 59.
3. J.R. Chelikowsky, N. Keskar, and N. Binggeli: "The Structural Properties of Silica Using Classical and Quantum Interatomic Forces," *Molecular Modeling of Minerals and Silicated Structures*, editors B. Silvi and Ph. D'Arco (Kluwer Academic Press, 1997), p.1.
4. N. Binggeli and J.R. Chelikowsky: "Ab Initio Pseudopotential Methods for Oxides: α-Quartz near the Amorphous Transition," *Quantum Theory of Real Materials*, J.R. Chelikowsky and S.G. Louie, editors, (Kluwer Press, 1996) p. 387.
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9. J.R. Chelikowsky and Y. Saad: "Grids in Space: The Electronic and Structural Properties of Clusters," *Chemical Design Automation News* **11**, 1 (1996).

10. J.R. Chelikowsky and N. Binggeli: "The Electronic and Structural Properties of Silica Using *Ab Initio* Pseudopotentials," *Structure and Imperfections in Amorphous and Crystalline SiO_2,*" R. Devine, J.-P. Duraud, and E. Dooryhée, editors, (Wiley, 2000), Chapter 8, p. 181.
11. J.R. Chelikowsky, N. Keskar, and N. Binggeli: "The Structural Properties of Silica Using Classical and Quantum Interatomic Forces," *Molecular Engineering* **6**, 1 (1996). [special issue to advertise forthcoming book].
12. "Computational and Theoretical Techniques for Materials Science," National Research Council, NRL Stragetic Series, (National Academy Press, 1995), NRC Panel Report.
13. J.R. Chelikowsky, S. Öğüt, I. Vasiliev, A. Stathopoulos, and Y.Saad: "Predicting the Properties of Semiconductor Clusters," *Theory of Atomic and Molecular Clusters*, J. Jellinek, editor,(Springer-Verlag, 1999) p. 136.
14. J.R. Chelikowsky: "The Electronic and Structural Properties of Semiconductor Clusters and Nanostructures," Proceedings of the 10th Physics Summer School, *Physics of Novel Materials*, Ed. M.P. Das (World Scientific, 1999) p. 1.
15. J.R. Chelikowsky: "The Pseudopotential-Density Functional Method Applied to Nanostructures," *J. Phys. D* **33**, R33 (2000).
16. J.R. Chelikowsky, Y. Saad, S.Öğüt, I. Vasiliev and A. Stathopoulos : "Electronic Structure Methods for Predicting the Properties of Materials: Grids in Space," *Computer Modeling of Materials Properties and Phenomena*: *phys. stat. sol. (b)*, **217**, 173 (2000). 6 pt
17. J.R. Chelikowsky:"The origin of the pseudopotential density functional method. Perspective on 'Microscopic theory of phase transformation and lattice dynamics of Si' - Yin MT, Cohen ML (1980) Phys Rev Lett **45**: 1004-1007" *Theoretical Chemistry Accounts*, **103**, 340 (2000).
18. J.R. Chelikowsky:"Quantum mechanics of condensed phases," *Encyclopedia of Chemical Physics and Physical Chemistry*, Institute of Physics. Editor-in-Chief: N. Spencer, (in press).
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21. J.R. Chelikowsky, L. Kronik, I. Vasiliev, M. Jain and Y. Saad, "Using Real Space Pseudopotentials for the Electronic Structure Problem," Editor, C. Le Bris, *Handbook of Numerical Analysis* (devoted to computational chemistry) (Elsevier, 2003), Volume X, p. 613
22. J.R. Chelikowsky: "Silicon in All its Forms," MRS Bulletin [Turnbull Lecture] **27**. 951 (2002).
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28. J.R. Chelikowsky and Y. Saad: "Electronic Structure of Clusters and Nanocrystals," *Handbook of Theoretical and Computational Nanotechnology*, Editors: Michael Rieth and Wolfram Schommers. (American Scientific) **8**, 797 (2006).
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33. J.R. Chelikowsky, Y. Saad, and I. Vasiliev: "Atoms and Clusters," in *Time Dependent Density Functional Theory*, edited by M. Marques, C.A. Ullrich, F. Nogueira, A. Rubio, K. Burke and E.K.U. Gross, "Lecture Notes in Physics" series. (Springer-Verlag, Heidelberg), Chapter 17, **706**, 259 (2006).
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Articles in Scientific Journals

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2. J.R. Chelikowsky, J.C. Phillips, M. Kamal, and M. Strauss: "Surface and Thermodynamic Interatomic Force Fields for Silicon Clusters and Bulk Phases," *Phys. Rev. Lett.* **62**, 292 (1989).
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9. A. Wall, Y. Gao, A. Raisanen, A. Franciosi, and J.R. Chelikowsky: "Electronic Structure of CdTe Revisited," *Phys. Rev.* B **43**, 4988 (1991).
10. J.R. Chelikowsky, H.E. King Jr., and J. Glinnemann: "Interatomic Potentials and the Structural Properties of Silicon Dioxide Under Pressure," *Phys. Rev.* B **41**, 10866 (1990).
11. J.R. Chelikowsky, and K.M. Glassford: "Classical Potentials for Covalent Solids and Clusters: Application to Silicon and Silicon Dioxide," *Mat . Res. Soc. Symp. Proc.* **193**, 65 (1990).
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13. J.R. Chelikowsky, H.E. King, Jr., N. Troullier, J.L. Martins, and J. Glinnemann: "Structural Properties of α-Quartz Near the Amorphous Transition," *Phys. Rev. Lett.* **65**, 3309 (1990).
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155. J.R. Chelikowsky: "Simulating Liquid GeTe," *MRS Symp. Proc.* **918**, 125 (2006).
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159. J.R. Chelikowsky: "The Role of Self-Purification and the Electronic Structure of Magnetically Doped Semiconductor Nanocrystals," *Phase Transitions* **79**, 739 (2006).
160. Y. Zhou, Y. Saad, M.L. Tiago, and J.R. Chelikowsky: "Parallel Self-Consistent-Field Calculations via Chebyshev-Filtered Subspace Acceleration," *Phys. Rev. E* **74**, 066704 (2006).

Invited Talks: Professional Society Meetings or Workshops

1. J.R. Chelikowsky: "Predicting the Properties of Materials with Pseudopotentials and Supercomputers", Materials Theory Conference, Princeton, NJ, March, 1989.
2. J.R. Chelikowsky: "The Electronic and Structural Properties of Silicon Clusters," Gordon Conference, Plymouth, NH, July 1989.
3. J.R. Chelikowsky: "Structure of Si_n (n=10-100) Clusters," March APS Meeting, Anaheim, CA, March 12-16, 1990.
4. J.R. Chelikowsky: "The Structure of Silicon and Silicon Dioxide from Interatomic Potentials" Materials Research Society Meeting, San Francisco, CA, April, 1990.
5. J.R. Chelikowsky: "Molecular Dynamics of C_{60} Formation from Isolated Hot Atoms," American Vacuum Society, Seattle, WA, November, 1991
6. J.R. Chelikowsky: "The Development of Orbital Radii as Modern Chemical Coordinates for the Prediction of Structural Trends in Alloys and Compound," The Minerals, Metals and Metallurgical Society, San Diego, CA, March, 1992.
7. J.R. Chelikowsky: "Pressure Dependence of the Electronic and Structural Properties of Crystalline SiO_2" Indianapolis Meeting of the American Physical Society, 16-20 March 1992. (Bull. APS **37**, 307 (1992)).
8. J.R. Chelikowsky, N. Binggeli and N.R. Keskar: "Structural and Elastic Behavior of Silica" Spring Meeting of the American Ceramic Society, Minneapolis, April, 1992.

9. J.R.Chelikowsky: "Structural Trends in Solids from Orbital Radii and Pseudopotential Methods," Workshop on Regularities, Classifications and Predictions of Advanced Materials, Lake Como, Italy, April, 1992.
10. J.R. Chelikowsky and Xiaodun Jing: "Nucleation of Carbon Clusters via Langevin Molecular Dynamics," Electrochemical Society Meeting, St. Louis, May, 1992.
11. J.R. Chelikowsky: "Order-Disorder Transformations and Elastic Anomalies in Silica," 4th Annual Workshop on Recent Developments in Electronic Structure Algorithms, Raleigh, NC, May, 1992.
12. J.R. Chelikowsky: "Structure of Covalent Clusters,"International Symposium on Small Particle and Inorganic Clusters (ISSPIC 6), Chicago, IL, September, 1992.
13. J.R. Chelikowsky: "Electronic and Structural of Properties of Silica," III Italian-Swiss Workshop on Computational Condensed Matter Physics, Sardinia, Italy, September, 1992.
14. J.R. Chelikowsky: "First Principles Methods for the Electronic and Structural Properties of Solid State Oxides" Fall Meeting of the Materials Research Society, Boston, November 1992.
15. J.R. Chelikowsky: "Mechanical Instabilities and the Amorphization of α-quartz Under Pressure," Sixth International Workshop on Computational Condensed Matter Physics," Trieste, Italy, January 1993.
16. J.R. Chelikowsky: "Quantum Langevin Molecular Dynamics Applied to Silicon Clusters," American Chemical Society Meeting, Denver, CO, April, 1993.
17. J.R. Chelikowsky: "Computing the Properties of Complex Materials," Italian-United States Workshop on Advanced Materials," Argonne National Laboratories, April, 1993.
18. J.R. Chelikowsky: "Modeling of Fullerenes," Sixth Scientific Computing Facility Users Group Meeting, "Computed Properties of Carbon Based Materials," Namur, Belgium, May, 1993.
19. J.R. Chelikowsky: "Amorphization of Quartz Under Pressure: Mechanisms from First Principles," AIRAPT and APS High Pressure Science and Technology Conference, Colorado Springs, CO, Bull. APS **39**, 1497 (1993).
20. J.R. Chelikowsky: "The Future of Computational Materials Science," Department of Energy workshop on electron microscopy, Tempe, AZ, October, 1993.
21. J.R. Chelikowsky, N. Troullier, and Y. Saad: "Higher Order Finite Difference Methods Applied to Electronic Structure Problems," Toward Teraflop Computing, Baton Rouge, LA, February, 1994.
22. J.R. Chelikowsky, N. Troullier, and Y. Saad: "Pseudopotentials and Symmetric Multiprocessing Algorithms for Computing the Properties of Liquid Semiconductors," March Meeting of the American Physical Society, Pittsburgh, PA, March 1994.
23. J.R. Chelikowsky: "Squeezing the Crystallinity Out of Solids: Pressure Induced Amorphization of Quartz," Conference on the Quantum Theory of Real Materials, Berkeley, CA, August, 1994.
24. J.R. Chelikowsky: "Quantum Simulations of Clusters Using the Finite-Difference Pseudopotential Method," International Symposium on Computational Molecular Dynamics, Minneapolis, MN, October, 1994.
25. J.R. Chelikowsky: "Simulating Clusters with REAL Forces in REAL Space," Workshop on Electronic Structure Theory, University of California at Davis, March, 1995.
26. J.R. Chelikowsky: "Elastic Anomalies and Pressure Induced Amorphization in Crystalline Silica," Computational Materials Science Conference, Morgantown, WV, May, 1995.

27. J.R. Chelikowsky: "Pressure Induced Amorphization and Memory Glasses in Quartz-like Materials," IV International Conference on Advanced Materials (ICAM-4), Cancun, Mexico, August, 1995.
28. J.R. Chelikowsky: "The Electronic and Structural Properties of Matter: From 'Bloch-Simons' to 'Ab Initio' Pseudopotentials," Aaron N. Bloch Symposium, Exxon Research and Engineering Company, NJ, October, 1995.
29. J.R. Chelikowsky, X. Jing and N. Binggeli: "Simulating the Properties of Clusters at Finite Temperatures with Finite Difference Methods," Materials Research Society, Boston, MA, November,1995.
30. J.R. Chelikowsky: "Grids in Space: Predicting the Electronic and Structural Properties of Localized Systems," CECAM Workshop, Lyon, France, July,1996.
31. J.R. Chelikowsky: Summer School on Physics of Novel Materials. Canberra, Australia, January, 1997.
32. J.R. Chelikowsky, "Quantum Confinement and Optical Gaps in Silicon Nanocrystals," International Materials Research Congress, Cancun, Mexico, September, 1997.
33. J.R. Chelikowsky: "Thermal properties and elastic anomalies in silica," CECAM Workshop, Lyon, France, September, 1997.
34. J.R. Chelikowsky: "Atomic Structure and Scanning Tunneling Microscopy of the As Vancancy on the GaAs (110) Surface," Materials Research Society, Boston, MA, November,1997.
35. J.R. Chelikowsky: "New Phase and Gradual Coordination Change in Silica Under Pressure," Materials Research Society, Boston, MA, November,1997.
36. J.R. Chelikowsky: "Predicting the Properties of Electronic Materials with Pseudopotentials and Supercomputers," Ninth CIMTEC World Forum on Materials Meeting, Florence, Italy, July, 1998.
37. J.R. Chelikowsky: "Optical Properties of Confined Systems," Dynamics of Clusters Workshop, sponsored by INT/ITAMP, Seattle Washington, July, 1998.
38. J.R. Chelikowsky: "The Evolution of Optical Properties in Nanostructures," Midwest Solid State Conference, Ames, Iowa, October, 1998.
39. J.R. Chelikowsky: "The Evolution of Optical Properties in Nanostructures," Ninth International Workshop on Computational Materials Science: Electronic Structure Theory and Simulations, Trieste, Italy, January, 1999.
40. J.R. Chelikowsky: "High Performance Algorithms for Predicting the Properties of Electronic Materials: Applications to Nanostructures," Workshop on Parallel Algorithms, Computational Efficiency and Multiscale Materials Simulations, New Orleans, April, 1999.
41. J.R. Chelikowsky:"Using TDLDA in Real Space: Applications to the Excitation Spectra and Collective Electronic Response in Clusters," Workshop on Time Dependent Local Density Approximation, Santa Barbara, April, 1999.
42. J.R. Chelikowsky:"The Evolution of Optical Properties in Nanostructures," International Conference on Advanced Materials, Beijing, China, June, 1999.
43. J.R. Chelikowsky:"Time Dependent Density Functional Theory Applied to the Optical Properties in Nanostructures," CECAM Workshop, Lyon, France, September,1999.
44. J.R. Chelikowsky:"Optical Excitations and Polarizabilities of Nanostructures," International Symposium on Clusters and Nanostructure Interfaces, Richmond, VA, October, 1999.
45. J.R. Chelikowsky: "Optical Excitations in Confined Systems," Conference of the Theory of Atomic and Molecular Clusters (TAMC-3), Berlin, Germany, October, 1999.

46. J.R. Chelikowsky: "A Coordinate Space Method for the Response Functions of Localized Systems," March Meeting of the American Physical Society, Bull. APS **45**, 874 (2000).
47. J.R. Chelikowsky: "Theory of Pseudopotentials," Spring College on Electronic Structure Approaches to the Physics of Materials, International Centre for Theoretical Physics, Trieste, Italy, May, 2000.
48. J.R. Chleikowsky: "Pressure Induced Amorphization in Quartz," 103rd Annual Meeting of the American Ceramic Society, April, 2001.
49. J.R. Chelikowsky: "Silicon in All its Forms," 2001 MRS Fall Meeting, Boston, MA, November, 2001. [Turnbull Award Lecture]
50. J.R. Chelikowsky: "Density Functional Theory from the Ground State to the Excited State," International Symposium of Atomic, Molecular and Solid State Theory, Sanibel, February, 2002. [Plenary Talk]
51. J.R. Chelikowsky: "Simulations of Semiconductor Liquids Using First Principles Molecular Dynamics," 15th Annual Workshop on *Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, Athens, GA, March 2002.
52. J.R. Chelikowsky: "Optical Excitations at the Nanostructure Scale," March Meeting of the American Physical Society, Indianapolis, IN, March 2002.
53. J.R. Chelikowsky: "Quantum Dots and Nanocrystals: Optical Excitations," 34th Great Lakes Regional Meeting of the American Chemical Society, Minneapolis, MN, June, 2002.
54. J.R. Chelikowsky: "Predicting the Properties of Liquid Semiconducors," Ninth CIMTEC World Forum on Materials Meeting, Florence, Italy, July, 2002. (presented by J. Derby)
55. J.R. Chelikowsky, M. Jain and L. Kronik: "Electronic Structure and Spin-Polarization of Mn-containing Dilute Magnetic III-V Semiconductors," American Vacuum Society, Denver, CO, November, 2002.
56. J.R. Chelikowsky: "Spin-Polarization and Electronic Structure of Mn Containing Dilute Magnetic III-V Semiconductors," Materials Research Society Fall 2002, Boston, MA, December 2002.
57. J.R. Chelikowsky: "Optical Excitations in Molecules, Clusters and Nanocrystals," Mardi Gras Conference: Frontiers of Grid Computing at the Nano-Bio Interface," Baton Rouge, LA, February 2003.
58. J.R. Chelikowsky: "Predicting the optical and electronic properties of semiconductors at the nanoscale," IGERT Nanoparticle Science and Engineering Summer Symposium, Minneapolis, MN, July, 2003.
59. J.R. Chelikowsky: "Optical properties and doping of semiconductor nanocrystals," Grand Challenges in Modeling the Assembly and Properties of Nanomaterials, DOE workshop at Argonne National Labs, August, 2003.
60. J.R. Chelikowsky: "Quantum confinement in nanocrystals: Optical excitations and doping. Computational Approaches towards the Electronics Properties of Quantum Workshop sponsored by DARPA-DSO, Chicago, September, 2003.
61. J.R. Chelikowsky: "Point Defects in Silicon: Modeling the Infinite with the Finite," Mardi Gras Conference: Materials and Modeling for Information Technology, Baton Rouge, LA, February 2004.
62. J.R. Chelikowsky: "Computational Methods for Predicting the Optical Properties of Matter at the Nanoscale," EC-NSF Workshop on Computational Methods in Materials Science, San Francisco, CA, April, 2004.

63. J.R. Chelikowsky; "Predicting the Optical and Structural Properties of Matter at the Nanoscale," Fourth SIAM Conference on Mathematical Aspects of Materials Science, Los Angeles, CA, May, 2004.
64. J.R. Chelikowsky: "Ab Initio Simulation of the Properties of Nanoclusters," 3rd International Conference on Computational Modeling and Simulation of Materials, Sicily, Italy, June, 2004.
65. J.R. Chelikowsky: "Numerical Methods for Predicting the Optical Properties of Nanocrystals," ACS/PRF Summer School on "Time-Dependent Density-Functional Theory and the Dynamics of Complex Systems," Santa Fe, NM, June, 2004.
66. J.R. Chelikowsky: "Atoms on the Move: Simulating the Properties of Semiconductor Liquids," Conference on Computational and Experimental Challenges, Los Angeles, CA, August, 2004.
67. J.R. Chelikowsky: "Optical Properties in Quantum Dots and Clusters Using Time Dependent Density Functional Theory," First-principles computational materials mini-school, Taipei, Taiwan, May, 2005.
68. J.R. Chelikowsky: "Magnetically Doped Quantum Dots," Grid Applications in Nanoscience, Nara, Japan, June 2005.
69. J.R. Chelikowsky: "Magnetism in Semiconductor Quantum Dots," Electronic structure workshop at Cornell, Ithaca, NY, June, 2005.
70. J.R. Chelikowsky: "Magnetic Doped Nanocrystals," International Symposium on Structure and Dynamics on the Nanometer Scale, Duisburg, Germany, November, 2005.
71. J.R. Chelikowsky: "Magnetic properties of Mn-doped semiconductor nanocrystals," 1st International Workshop on Doping Semiconductor Nanostructures, Washington DC, January, 2006.
72. J.R. Chelikowsky: "Theory of Optical Properties of Nanocrystals," DOE Workshop, Orlando, FL, February, 2006.
73. J.R. Chelikowsky: "Nanocrystals, Nanowires and the Role of Quantum Confinement," March Meeting of the American Physical Society, Baltimore, MD, March, 2006. [David Adler Award].
74. J.R. Chelikowsky: "Local Structure of Liquid GeTe via *Ab Initio* Molecular Dynamics Simulation," Materials Research Society Spring Meeting, San Francisco, CA, April, 2006.
75. J.R. Chelikowsky: "Optical and Magnetic Properties in Nanocrystals," Workshop, Molecular Foundry, Lawrence Berkeley Laboratory, Berkeley, CA, May, 2006.
76. J.R. Chelikowsky: "The Evolution of Optical and Magnetic Properties in Nanocrystals," Conference on Computational Physics, Gyeongju, Korea, August, 2006. [Plenary talk]
77. J.R. Chelikowsky: "Predicting Electronic Properties at the Nanoscale," US-Ireland R&D Nanotechnology Workshop, Belfast, Ireland, October, 2006.
78. J.R. Chelikowsky: "Algorithms for Predicting the Optical and Magnetic Properties of Nanocrystals," Workshop on Computational Methods for Nanoscale Systems, Hong Kong, China, December, 2006. [Keynote talk]
79. J.R. Chelikowsky: "Evolution of Magnetism in Iron from the Atom to the Crystal," Taiwan-US Joint Workshop on Frontiers in Nanoscience, Taipei, Taiwan, December, 2006.

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